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## A large eddy simulation scheme for turbulent reacting flows

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### 1. Motivation and objectives

Turbulent reacting flow has been an important problem and has attracted much attention from researchers in a variety of science and engineering disciplines. Despite intense research activity, however, much remains to be done in this field (O'Brien 1980; Pope 1985, 1990). One of the key issues in engineering application is to employ the existing models and techniques to develop a relatively simple numerical scheme for simulating complicated reacting flow systems.

Several approaches have been introduced to overcome the closure problems encountered in turbulent reacting flow simulations. Among them, the probability density function (PDF) method provides a closed form representation for the chemical source terms (O'Brien 1980; Pope 1985); for this reason it has become a preferred choice. However, the scalar PDF does not contain information concerning the transporting velocity field and the interactions between the scalar and velocity fields that has to be provided by supplementary turbulent transport and mixing models in reacting flow simulations.

The recent development of the dynamic subgrid-scale (SGS) model (Germano 1992; Germano *et al* 1991; Ghosal *et al* 1992) has provided a consistent method for generating localized turbulent mixing models and has opened up great possibilities for applying the large eddy simulation (LES) technique to real world problems. Given the fact that the direct numerical simulation (DNS) can not solve for engineering flow problems in the foreseeable future (Reynolds 1989), the LES is certainly an attractive alternative. It seems only natural to bring this new development in SGS modeling to bear on the reacting flows.

The major stumbling block for introducing LES to reacting flow problems has been the proper modeling of the reaction source terms. Various models have been proposed, but none of them has a wide range of applicability. For example, some of the models in combustion have been based on the flamelet assumption (Kerstein *et al* 1988; Trouvé & Poinso 1992), which is only valid for relatively fast reactions. Some other models have neglected the effects of chemical reactions on the turbulent mixing time scale (Valiño & Gao 1992), which is certainly not valid for fast and non-isothermal reactions (Vervisch 1993).

The PDF method can be usefully employed to deal with the modeling of the reaction source terms. In order to fit into the framework of LES, a new PDF, the large eddy PDF (LEPDF), is introduced. This PDF provides an accurate representation for the filtered chemical source terms and can be readily calculated in the simulations. The details of this scheme are described below.

## 2. Accomplishments

### Large eddy PDF

The large eddy fields, which are explicitly simulated in the LES, can be obtained by filtering the true fields with certain filters  $G$  (Germano 1992; Rogallo & Moin 1984); namely,

$$\bar{A}(\mathbf{x}, t) = \int_{-\infty}^{\infty} A(\mathbf{x}', t) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'.$$

Among the commonly used filters, we are particularly interested in those that are localized in physical space, such as the local volume average (Schumann 1975) and the Gaussian filters (Leonard 1974), since they describe local averaged effects. For reasons that will become clear later, we choose only these positive definite filters.

By applying a filter of size  $\Delta$ , which is generally the mesh size in LES, the Navier-Stokes equation can be written as

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = \nu \nabla^2 \bar{u}_i - \nabla \bar{p} - \frac{\partial \tau_{ij}}{\partial x_j}. \quad (1)$$

Here  $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$  is the SGS stress and is normally modeled by the eddy-viscosity model originally proposed by Smagorinsky (Smagorinsky 1963):

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2C \Delta^2 |\bar{S}| \bar{S}_{ij}, \quad (2)$$

where  $S_{ij}$  is the strain rate tensor

$$S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

and  $|\bar{S}| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$ .

The same type of filter with larger size  $\tilde{\Delta} > \Delta$  can be applied to the same equation. The resulting SGS stress can be represented by

$$T_{ij} = \overline{\tilde{u}_i \tilde{u}_j} - \tilde{u}_i \tilde{u}_j.$$

If the filters are well behaved ones such as the Gaussian filters, we will have the following convolution relation

$$G(\mathbf{x} - \mathbf{x}', l) = G(l_1) * G(l_2) = \int G(\mathbf{x} - \mathbf{x}_1, l_1) G(\mathbf{x}_1 - \mathbf{x}', l_2) d\mathbf{x}_1. \quad (3)$$

Take the Gaussian filter as an example; it can be shown that  $l^2 = l_1^2 + l_2^2$ . It is obvious from (3) that  $\tilde{A} = \hat{A}$ , where “ $\hat{A}$ ” is the filtering performed by the “gap filter” between  $\tilde{\Delta}$  and  $\Delta$ . The Germano identity (Germano 1992)

$$T_{ij} - \hat{\tau}_{ij} = L_{ij} = \overline{\tilde{u}_i \tilde{u}_j} - \hat{u}_i \hat{u}_j, \quad (4)$$

where the right hand side can be explicitly evaluated from the LES field, can then be used to calculate the local coefficient  $C$  for the Smagorinsky model (Germano *et al* 1991; Moin 1991; Lilly 1992).

A similar method can be applied to the turbulent scalar field  $\psi$ , which is governed by

$$\frac{\partial \psi}{\partial t} + u_j \frac{\partial \psi}{\partial x_j} = D \nabla^2 \psi + \omega(\psi(\mathbf{x}, t)). \quad (5)$$

Its large eddy counter-part can be written as

$$\frac{\partial \bar{\psi}}{\partial t} + \bar{u}_j \frac{\partial \bar{\psi}}{\partial x_j} = D \nabla^2 \bar{\psi} - \frac{\partial}{\partial x_j} (\overline{u_j \psi} - \bar{u}_j \bar{\psi}) + \bar{\omega}(\mathbf{x}, t). \quad (6)$$

Similar eddy-viscosity type models can be developed for the scalar field (Moin *et al* 1991), namely

$$\overline{u_j \psi} - \bar{u}_j \bar{\psi} = -D_s \frac{\partial \bar{\psi}}{\partial x_j}, \quad (7)$$

where  $D_s$  can again be obtained through the dynamic procedure described above.

The major problem is to find a suitable SGS model for the reaction source term  $\omega(\psi)$ . Noticing that

$$\bar{\omega}(\mathbf{x}, t) = \int_{-\infty}^{\infty} \omega(\psi(\mathbf{x}', t)) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}' = \int [d\phi \omega(\phi) \int_{-\infty}^{\infty} \rho(\phi; \mathbf{x}', t) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'], \quad (8)$$

where

$$\rho(\phi; \mathbf{x}, t) = \delta(\phi - \psi(\mathbf{x}, t))$$

is the fine-grain function, it is clear that once

$$P_L(\phi; \mathbf{x}, t) = \int_{-\infty}^{\infty} \rho(\phi; \mathbf{x}', t) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}' \quad (9)$$

is known, the filtered equation for the scalar field  $\psi$  is closed. For positive-definite filters, it can be shown that  $P_L$  has all the properties a PDF should have. We define it as the large eddy PDF. It is a generalization of the existing PDF concept.

In fact, for a homogeneous field, where the ensemble average can be replaced by the space average, the traditional PDF (O'Brien 1980; Pope 1985) can be recovered from our definition if a volume average filter is applied to a large enough space volume. For more general cases,  $P_L$  can be regarded as a weighted average of all contributions from the neighboring field points, depending on how far they are from the observation point.

The governing equation for  $P_L$  can be derived following the standard procedure (O'Brien 1980; Pope 1985). It can be shown that

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = -\frac{\partial}{\partial \phi} [(D \nabla^2 \psi + \omega) \rho]. \quad (10)$$

Applying the filter on both hand sides of (10), we get

$$\frac{\partial P_L}{\partial t} + \bar{\mathbf{u}} \cdot \nabla P_L = -\frac{\partial}{\partial \phi} [D(\overline{\rho \nabla^2 \psi}) + \omega(\phi)P_L] - \frac{\partial}{\partial x_j} (\bar{u}_j \bar{\rho} - \bar{u}_j \bar{\rho}). \quad (11)$$

The last term on the RHS of (11) can again be modeled by the eddy viscosity assumption. Since  $\rho$  is controlled by the underlying process  $\psi$ , the  $D_s$  obtained for  $\psi$  is equally applicable for  $\rho$  (Jiang & O'Brien 1991). A brief proof follows.

Suppose the eddy-viscosity for  $P_L$  is  $D_p$ . Note that

$$\overline{f(\psi)} = \int \phi P_L(\phi) d\phi.$$

It can be shown, by multiplying  $\phi$  on both sides of equation (11) and integrating over the composition space after inserting

$$\bar{u}_j \bar{\rho} - \bar{u}_j \bar{\rho} = -D_p \frac{\partial P_L}{\partial x_j}$$

that

$$\frac{\partial \bar{\psi}}{\partial t} + \bar{u}_j \frac{\partial \bar{\psi}}{\partial x_j} = D \nabla^2 \bar{\psi} + \frac{\partial}{\partial x_j} (D_p \frac{\partial \bar{\psi}}{\partial x_j}) + \bar{\omega}(\mathbf{x}, t).$$

Comparing this equation to equations (6) and (7), it is obvious that  $D_p = D_s$ .

It can be shown that

$$\overline{(\rho \nabla^2 \psi)} = E_L \{ \nabla^2 \psi | \phi \} P_L(\phi).$$

If  $A$  and  $B$  are composition space representation of the fields  $a(\mathbf{x})$  and  $b(\mathbf{x})$ , then  $E_L$  is defined by

$$E_L \{ A | B \} P_L(B) = \int A P_L(A, B) dA$$

and

$$P_L(A, B) = \int \delta(A - a(\mathbf{x}')) \delta(B - b(\mathbf{x}')) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'.$$

$E_L \{ A | B \}$  can be interpreted as the average of  $A$ , weighted by  $G(\mathbf{x}' - \mathbf{x})$ , over the spots where  $b(\mathbf{x}') = B$ . The modeling of this term is generally difficult, as we have experienced in the traditional PDF approach. However, the fundamental physics expressed by this term remains the same - it represents the enhancement of diffusion by turbulent fluctuations. Therefore, models analogous to those used in the traditional PDF can be used to close this term. For example, if the LMSE model (O'Brien 1980) were used, we would have

$$E_L \{ \nabla^2 \psi | \phi \} \sim -\frac{1}{\tau_L} (\phi - \bar{\psi}) + D \nabla^2 \bar{\psi},$$

where  $1/\tau_L \propto (D + D_s)$ . After substituting this relation into (11), it can be shown that (11) recovers (6). Therefore, this relaxation model is adequate if one is only interested in the large eddy field.

Equation (11), supplemented by the above closure models, can be solved using the well established Monte-Carlo techniques for the scalar PDF (Pope 1981, 1985). A few advantages of this simulation scheme can be immediately identified. First, a general model for the chemical source term is developed based on the PDF. It, in principle, applies to all kinds of reactions and does not require any artificial pre-assumptions. Secondly, the interactions between chemical reaction and turbulent mixing are embedded in the current model – the effects of reaction on turbulent mixing are reflected in  $D_s$  through the dynamic procedure. Thirdly, the LES provides the flexibility of resolving a certain range of large scale structures while modeling the contributions from the rest of the scales. It can be applied to a wide range of problems with different degrees of resolution depending on the available resources. Moreover, it may be worth mentioning that the Monte-Carlo simulation for scalar PDF is a well established technique while LES has shown great potential with the introduction of the dynamic SGS model. The outlook for applying the proposed scheme seems to be promising. We intend to apply the scheme described above to reactive flow problems in a number of turbulent flows, such as in homogeneous flows, for which DNS results are available.

#### *A consistency condition for SGS model*

There are, however, certain problems that should be further investigated. Correctly modeling turbulent mixing in the PDF formulation has been a long-standing problem which surely deserves more attention (Gao 1993). The consistent determination of the eddy viscosity in the LES is another such problem.

Several different consistency conditions should be considered in calculating the eddy viscosity. First, the eddy viscosity is localized; namely, it is a function of both space and time. It can not be taken freely out of the space filter; therefore, it cannot be evaluated by simple algebraic procedures. A variational approach (Ghosal *et al* 1992), which leads to an integral equation for the coefficient  $C$ , and a differential equation approach, which will be described below, have been developed to overcome this problem. Another problem is that there is no reason to believe that the eddy viscosity should be the same on both the cut-off ( $\Delta$ ) and the test ( $\tilde{\Delta}$ ) filter levels. Since the equation for  $C$  constitutes an over-determined problem (six equations for two  $C$  in the case of velocity, if different model coefficients are assumed for different filter levels), the least mean square estimate technique can be used to evaluate these different model coefficients at different levels (Moin 1991; Lilly 1992). To use the variational approach, two integral equations will have to be solved. It could be numerically very intense to do so.

In fact, if  $\Delta$  and  $\tilde{\Delta}$  are in different scale ranges, there is no reason even to believe that  $T_{ij} \sim T_{ij}(\hat{S}_{ij})$  and  $\tau_{ij} \sim \tau_{ij}(\bar{S}_{ij})$  will have the same functional form. It is, therefore, helpful to imagine that the cut-off and the test levels are brought closer and closer to each other. In this limiting process, we can be assured that  $T_{ij}$  and  $\tau_{ij}$  will have the same functional form and that the coefficients  $C$  at different levels

will approach each other.

A formal procedure can be performed in this limiting case. For simplicity, we will omit the bar in  $\bar{u}$  in the following derivations.

We assume that the gap between the cut-off and the test filters are represented by  $\epsilon$ . As the gap between two filters narrows ( $\epsilon \rightarrow 0$ ),  $G(\mathbf{x}' - \mathbf{x}, \epsilon)$  becomes more "concentrated". In fact,

$$\lim_{\epsilon \rightarrow 0} G(\mathbf{x}' - \mathbf{x}, \epsilon) = \delta(\mathbf{x}' - \mathbf{x}).$$

Let

$$\theta = \int (\mathbf{x}_1 - \mathbf{x})^2 G(\mathbf{x}_1 - \mathbf{x}, \epsilon) d\mathbf{x}_1, \quad (12)$$

it is obvious that  $\lim_{\epsilon \rightarrow 0} \theta = 0$ .

For simplicity, we will only consider symmetric filters, i.e.  $G = G(|\mathbf{x}_1 - \mathbf{x}|)$ . However, this method is not restricted to symmetric filters.

Under symmetric conditions, we have

$$\hat{u}(\mathbf{x}) = \int u G(\mathbf{x}_1 - \mathbf{x}, \epsilon) d\mathbf{x}_1 = u(\mathbf{x}) + \frac{\theta}{2} \nabla^2 u + O(\theta^2). \quad (13)$$

Obviously,

$$L_{ij} = \theta \nabla u_i \cdot \nabla u_j + O(\theta^2). \quad (14)$$

Similarly, for the Smagorinsky type of SGS model, we have

$$\begin{aligned} T_{ij} - \hat{\tau}_{ij} &= \theta \left[ -2C\Delta^2 \left( \alpha \frac{|S|}{\Delta^2} S_{ij} + \frac{|S|}{2} \nabla^2 S_{ij} + \frac{S_{kl} \nabla^2 S_{kl}}{|S|} S_{ij} \right) \right. \\ &\quad \left. + \Delta^2 \nabla^2 (C|S|S_{ij}) + \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_l} \frac{\partial u_k}{\partial x_l} \right] + O(\theta^2), \end{aligned} \quad (15)$$

where we have used the relation  $\tilde{\Delta}^2 = \Delta^2 + \alpha\theta^2$ . For Gaussian filters,  $\alpha = 1$ .

Substituting both (14) and (15) into the Germano identity (4) and taking the limit  $\epsilon \rightarrow 0$ , we have

$$\begin{aligned} &-2C\Delta^2 \left( \alpha \frac{|S|}{\Delta^2} S_{ij} + \frac{|S|}{2} \nabla^2 S_{ij} + \frac{S_{kl} \nabla^2 S_{kl}}{|S|} S_{ij} \right) + \Delta^2 \nabla^2 (C|S|S_{ij}) \\ &= \nabla u_i \cdot \nabla u_j - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_l} \frac{\partial u_k}{\partial x_l}. \end{aligned} \quad (16)$$

This equation, when properly contracted, can be used to solve for the local model coefficient,  $C$ . Clearly, this procedure can be equally useful if different functional forms for  $S_{ij}$  and  $\tau_{ij}$  are chosen.

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